SUPPORTING INFORMATION

Structural characterization of suppressor lipids by high-resolution mass spectrometry

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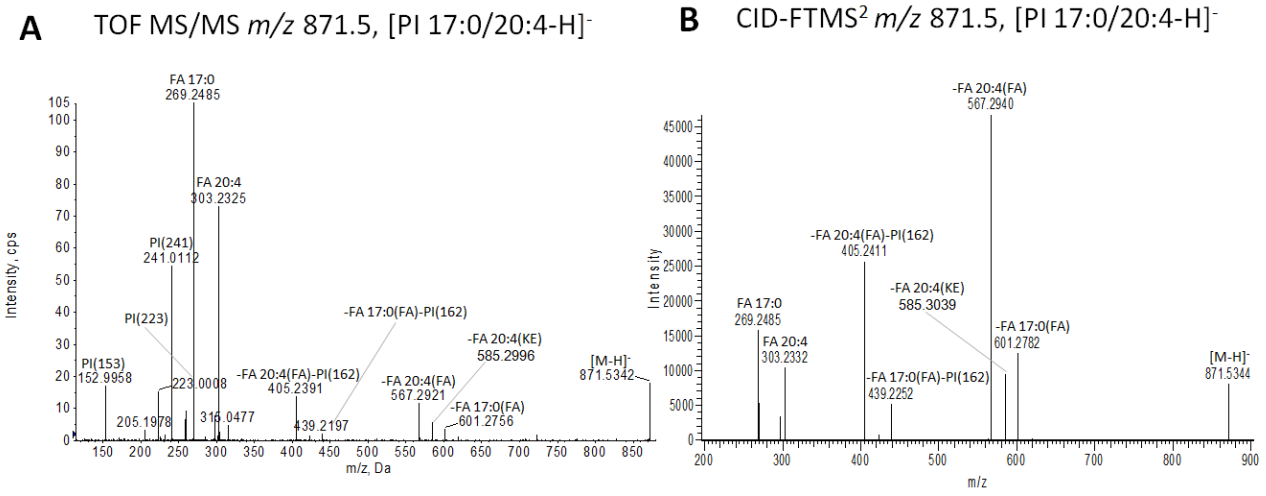

Figure S1. Structural characterization of synthetic PI 17:0/20:4. (A) TOF MS/MS spectrum of *m/z* 871.5 ([PI 17:0/20:4-H]$^-$) acquired using CE at 64 eV. (B) FTMS^2 spectrum of *m/z* 871.5 ([PI 17:0/20:4-H]$^-$) acquired using CID and CE at 34%.

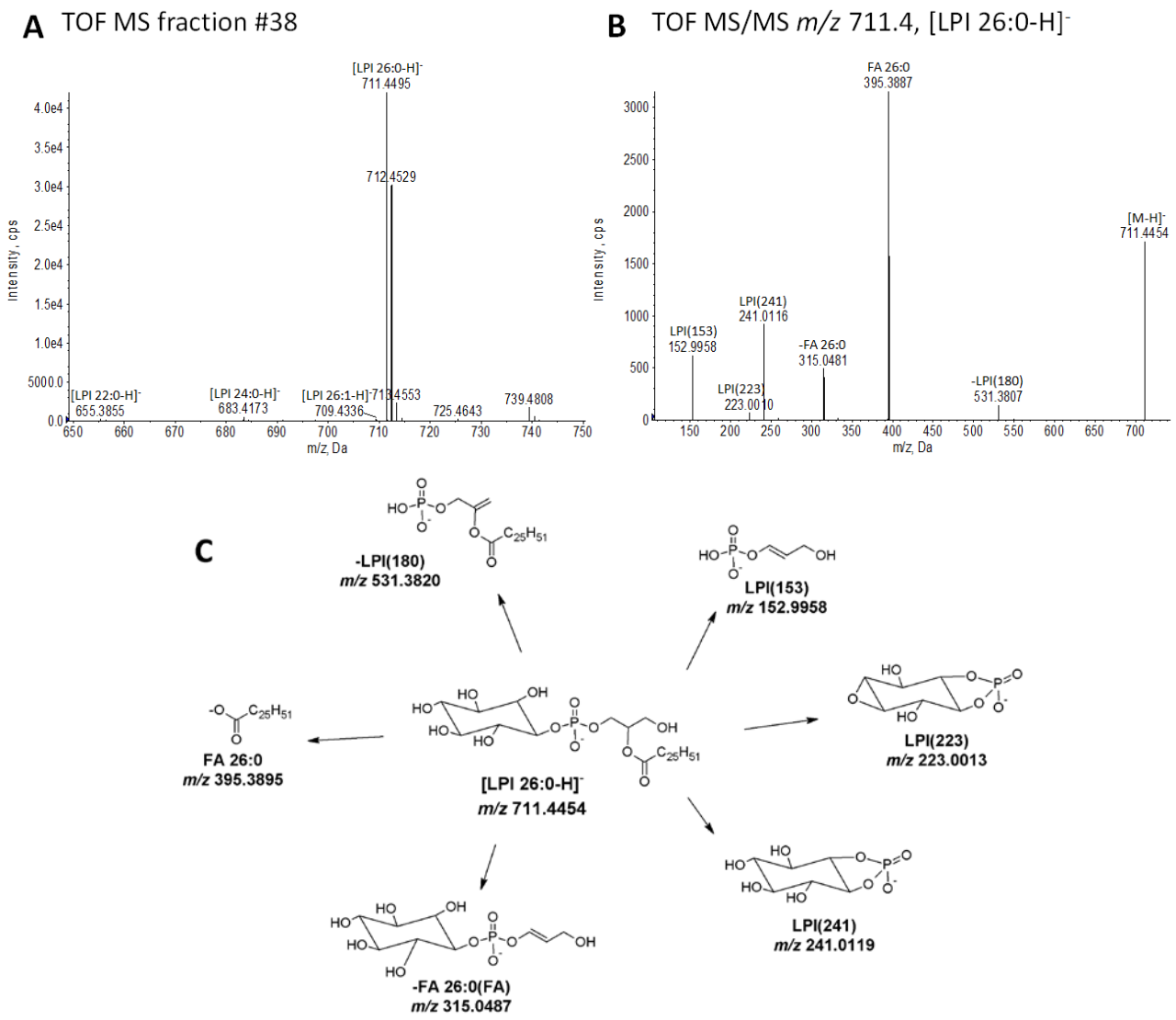

Figure S2. Structural characterization of LPI 26:0. (A) FTMS spectrum of fraction #38. (B) TOF MS/MS spectrum of *m/z* 711.4 ([LPI 26:0-H]$^-$). (C) Tentative structures and predominant fragmentation pathways of LPI 26:0. Specified *m/z* values are calculated based on the chemical composition of depicted structures.

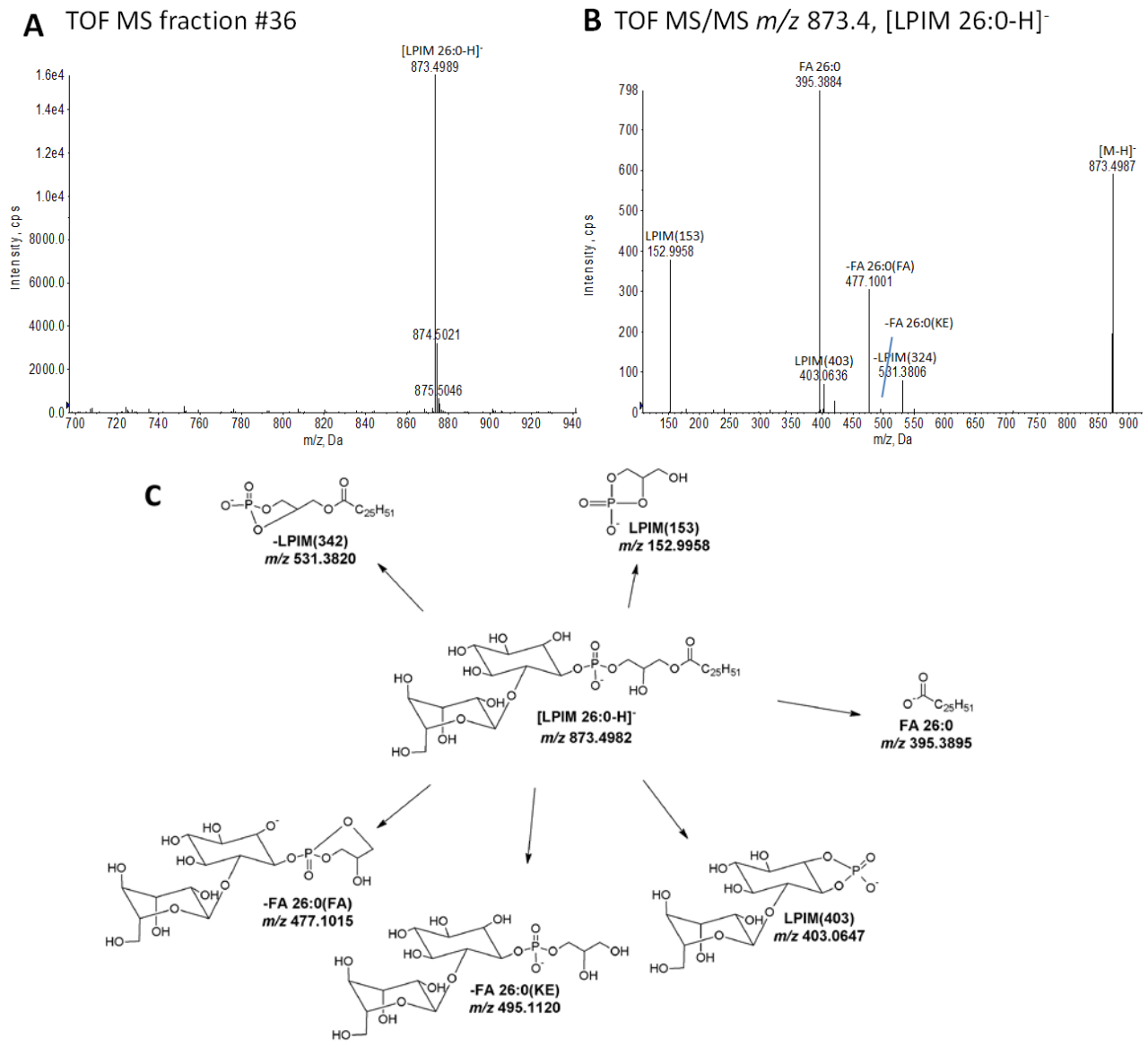

Figure S3. Structural characterization of LPIM 26:0. (A) FTMS spectrum of fraction #36. (B) TOF MS/MS spectrum of *m/z* 873.5 ([LPIM 26:0-H]$^-$). (C) Tentative structures and predominant fragmentation pathways of LPIM 26:0. Specified *m/z* values are calculated based on the chemical composition of depicted structures.

Figure S4.

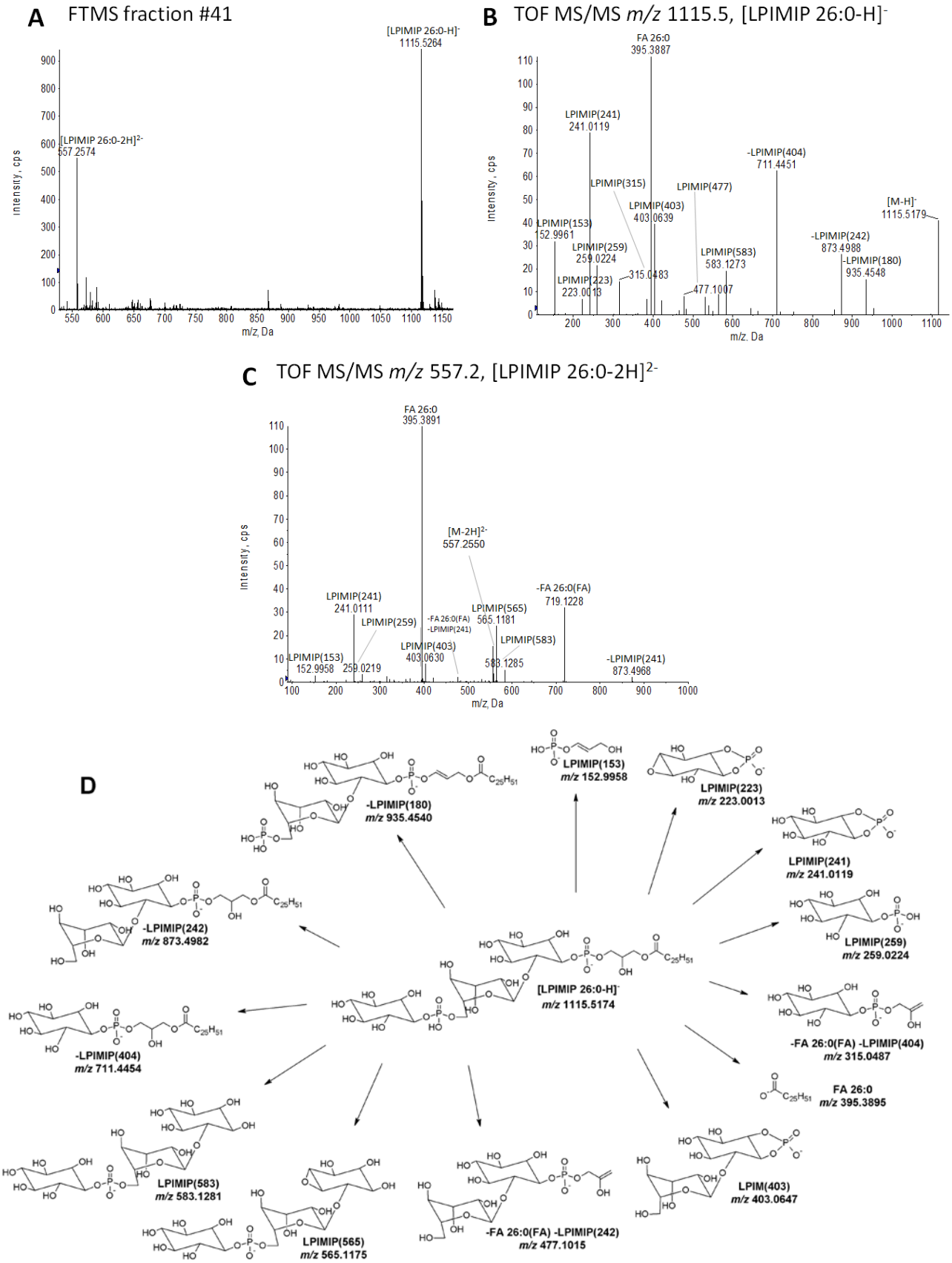
A FTMS fraction #41
[LPIMIP 26:0-H]-
1115.5264
[LPIMIP 26:0-2H]2-
557.2574
Intensity, cps
m/z, Da
B TOF MS/MS m/z 1115.5, [LPIMIP 26:0-H]-
FA 26:0
395.3887
LPIMIP(241)
241.0119
-LPIMIP(404)
711.4451
LPIMIP(315)
LPIMIP(477)
LPIMIP(403)
403.0639
[M-H]-
1115.5179
LPIMIP(153)
152.9961
LPIMIP(259)
259.0224
LPIMIP(583)
583.1273
-LPIMIP(242)
873.4988
-LPIMIP(180)
935.4548
315.0483
LPIMIP(223)
223.0013
477.1007
C TOF MS/MS m/z 557.2, [LPIMIP 26:0-2H]2-
FA 26:0
395.3891
[M-2H]2-
557.2550
-FA 26:0(FA)
719.1228
LPIMIP(241)
241.0111
LPIMIP(259)
-FA 26:0(FA)
-LPIMIP(241)
LPIMIP(565)
565.1181
LPIMIP(403)
403.0630
LPIMIP(583)
583.1285
LPIMIP(153)
152.9958
259.0219
-LPIMIP(241)
873.4968
D
-LPIMIP(180)
m/z 935.4540
LPIMIP(153)
m/z 152.9958
LPIMIP(223)
m/z 223.0013
LPIMIP(241)
m/z 241.0119
LPIMIP(259)
m/z 259.0224
-LPIMIP(242)
m/z 873.4982
[LPIMIP 26:0-H]-
m/z 1115.5174
-FA 26:0(FA) -LPIMIP(404)
m/z 315.0487
-LPIMIP(404)
m/z 711.4454
FA 26:0
m/z 395.3895
LPIMIP(583)
m/z 583.1281
LPIM(403)
m/z 403.0647
LPIMIP(565)
m/z 565.1175
-FA 26:0(FA) -LPIMIP(242)
m/z 477.1015

Figure S4 (continued).

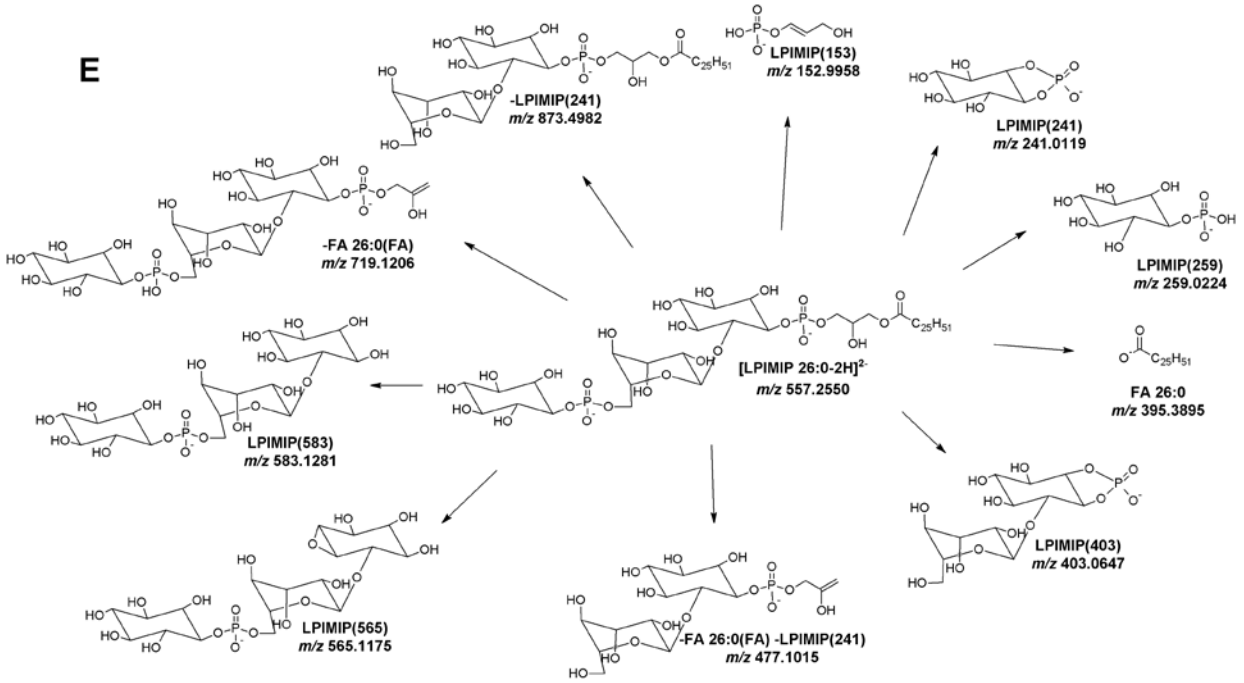

Figure S4. Structural characterization of LPIMIP 26:0. (A) FTMS spectrum of fraction #41. (B) TOF MS/MS spectrum of *m/z* 1115.5 ($[LPIMIP\ 26:0\text{-}H]^-$). (C) TOF MS/MS spectrum of *m/z* 557.2 ($[LPIMIP\ 26:0\text{-}2H]^{2-}$). (D) Tentative structures and predominant fragmentation pathways of singly charged LPIMIP 26:0. (E) Tentative structures and predominant fragmentation pathways of doubly charged LPIMIP 26:0. Specified *m/z* values are calculated based on the chemical composition of depicted structures.